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ASC Directions in Machine Learning @LANL

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Machine Learning For ASC

Goal: To find ways to impact ASC work in the IC, V&V and PEM.

In particular *in-line* ML as opposed to post processing.



We have more mature work in the CSSE/FOUS area of ASC

Existing work in Machine Learning

- **Image and Video based work (Dwave, Neuro, GPU, CPU)**
 - Sparse Coding/Compressive Sensing of Radiographic Sequences
 - Predicting Fractures with Sparse Coding
- **Infrastructure to run ML kernels on system log data**
- **Machine Learning on System Logs**
 - Developing tool to use temporal characteristics of system logs (including telemetry / environmental data) for anomaly detection
 - Developing tool to predict job outcome based on early warnings from system logs
 - Test developed DRAM fault mitigation tool on Trinity supercomputer

New starts for Machine Learning in Mid FY18

- **ML for Coarse-Graining and Structure Tagging for Fluid Simulations**
 - First goal - Predict future state of system by learning exact relationship of data at future times from data at previous times using data from simulation. Using Burger's equation.
 - Second goal - Learn approximate relationship of data at future times from coarse grained data at previous times using data from simulation

A Machine Learning Approach to Coarse-Graining and Structure Tagging for Fluid Simulations

Basic Idea: Learn how to integrate a fluid equation from simulation data

$$u_j^{n+1} = f(\dots, u_{j-1}^n, u_j^n, u_{j+1}^n, \dots)$$

The diagram illustrates the components of the equation $u_j^{n+1} = f(\dots, u_{j-1}^n, u_j^n, u_{j+1}^n, \dots)$. A point labeled "Given data" has two arrows originating from it. One arrow points diagonally upwards and to the right, ending at the variable u_j^{n+1} on the left side of the equation. The other arrow points diagonally upwards and to the right, ending at the function f in the middle of the equation. A vertical line segment connects the function f to the text "Learn dependence" located below it.

Method for learning dependence: Machine learning - use optimization to find parameters of a general non-linear transformation

New starts for Machine Learning in Mid FY18 (cont.)

- **ML for Multi-scale Materials**

- *On-line* or *active* machine learning using inexpensive coarse-scale models combined in a single application code with expensive fine-scale models to simulate physical phenomena scalably across multiple time and length scales.
- PEM/ATDM effort

- **Developing ideas in V&V and Data reduction/analysis.**

Predicting Fractures with Sparse Coding



Goal: Predict unseen frames of a fracture propagation simulation by leveraging the latent representation learned by an unsupervised sparse autoencoder

Example frame from fracture dataset

Predicting Fractures with Sparse Coding

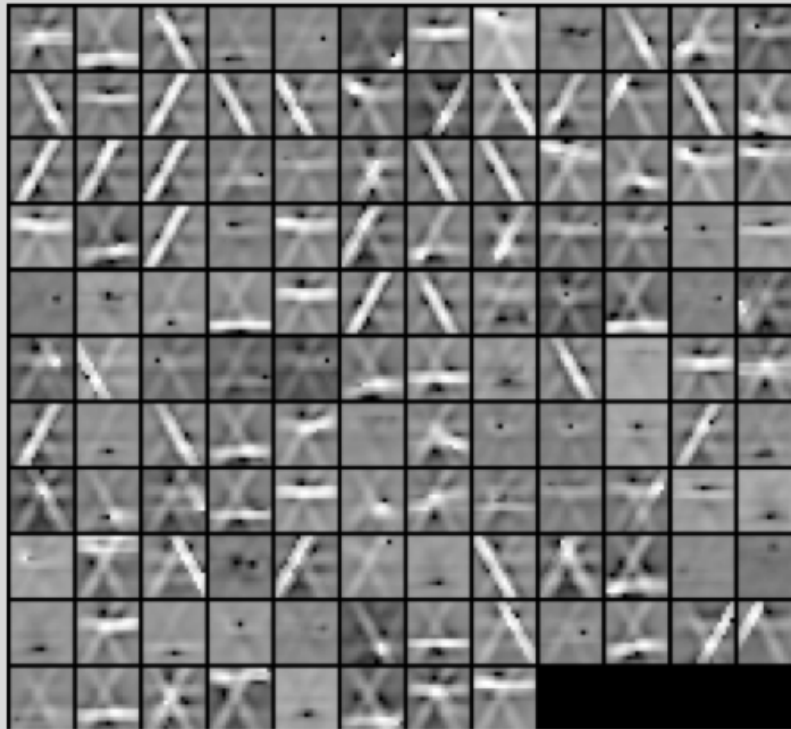
Process: Train a sparse code on 12 difference frames of fracture propagation. Train a deep network to predict the full 24 frame sequence, using the sparse code as input.

Left: Actual data
Right: Predicted data



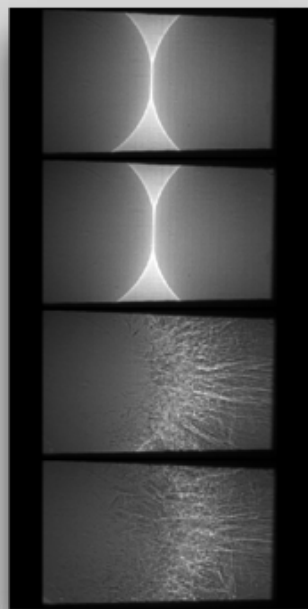
Predicting Fractures with Sparse Coding

Deep network weight visualization:

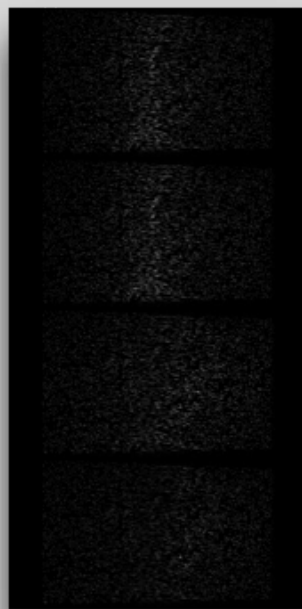


Reconstruct an X-ray image from random pixel sampling

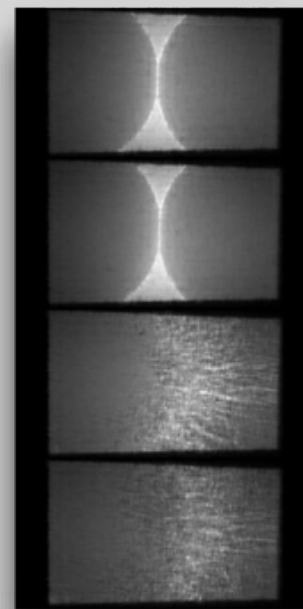
Masks cover 90% of pixels



(a) originals



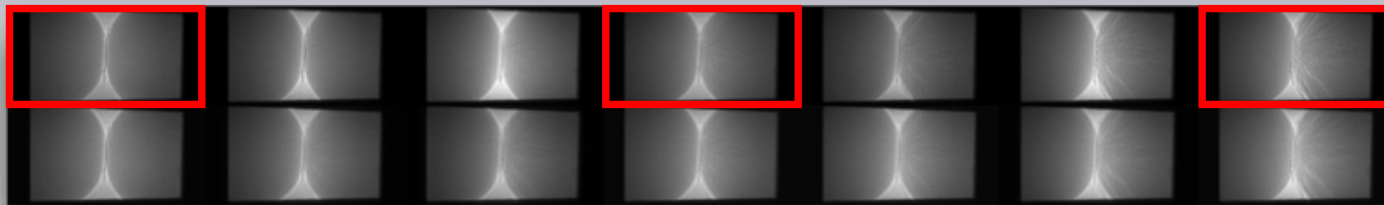
(b) masked samples



(c) reconstructions

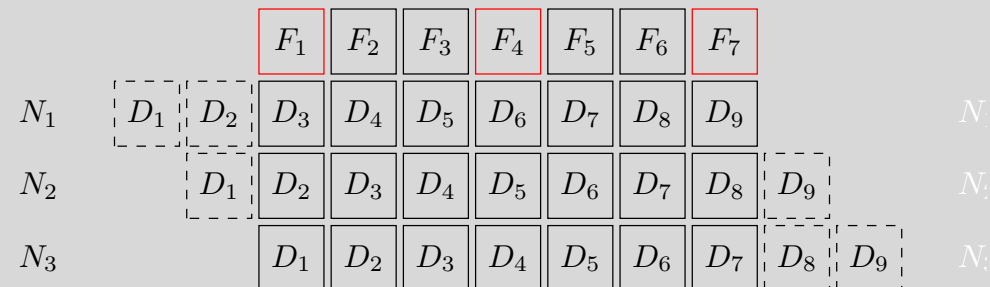
Z. Wang, O. Iaroshenko, S. Li, T. Liu, N. Parab, W. W. Chen, P. Chu, G. Kenyon, R. Lipton, and K.-X. Sune. Random on-board pixel sampling (ROPS) X-ray camera, Journal of Instrumentation (submitted)

Reconstruct intermediate frames (increase frame-rate)

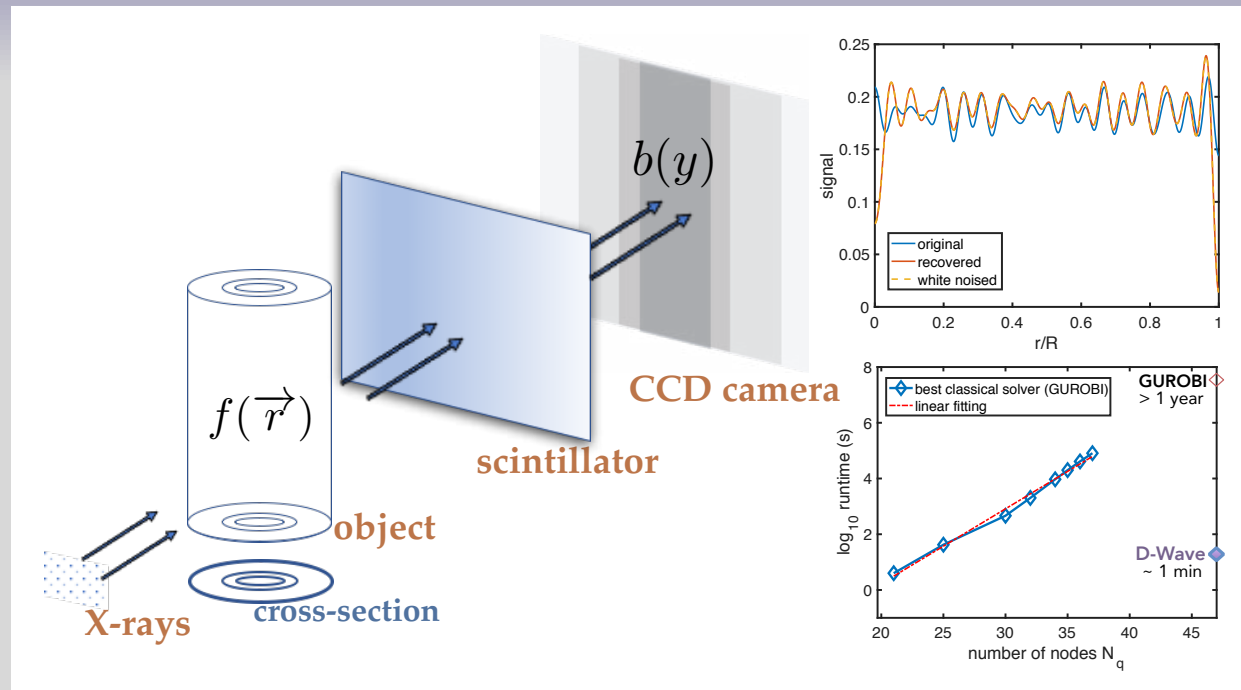


Top row: original frames, bottom row: reconstructed frames

Sparse coding algorithm can see only every third frame (red boxes)



Radiographic Inference



Nguyen, N.T.T., Larson, A.E., Kenyon, G.T., [Implementation of a compressive sensing protocol on the quantum D-Wave 2X for inferring radial density profiles from synthetic radiographic images](#), (submitted)

Nguyen, N.T.T., Larson, A.E., and Kenyon, G.T., [Generating sparse representations using quantum annealing: Comparison to classical algorithms](#), *IEEE International Conference on Rebooting Computing (ICRC)*, 2017 (in press)